

Using Machine Learning for Modelling Dynamic Operation of CO₂ Capture considering Different Application Requirements

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ABSTRACT

Accurate dynamic modelling of CO₂ capture is essential for real time process integration, control and optimization. This work aims to investigate the feasibility of using machine learning (ML) methods for different purposes of dynamic modelling of CO₂ capture. Since the development of ML models relies on the selection of input features, the key input parameters are first reviewed and determined based on requirements of various dynamic model applications. Four cases are covered in this work: system identification for control development, system monitoring and diagnosis, operation optimization and system performance assessment. Three ML methods, Informer, Long Short-Term Memory (LSTM) and Backpropagation Neural Network (BPNN), are used. The data needed for ML model development are generated by using a validated physical dynamic model developed in Aspen HYSYS Dynamics, based on real data of flue gas obtained from a waste fired combined heat and power plant. It was found that with selected input parameters, ML models can achieve high accuracy for all cases, with mean absolute percentage errors (MAPEs) less than 5%. No single model outperforms the others across all cases.

Keywords: dynamic modelling of CO₂ capture, machine learning (ML) approaches, combined heat and power (CHP) plants, application cases, model selection

NONMENCLATURE

Abbreviations

APE	absolute percentage error
BA-ELM	bootstrap aggregated extreme learning machine
BA-NN	bootstrap aggregated-neural network
BPNN	back propagation neural network

CHP	combined heat and power
DBN	deep belief network
FG	flue gas
INN	integral neural network
LSTM	long short-term memory network
MAPE	mean absolute percentage error
MAE	mean absolute error
MEA-CA	MEA based chemical absorption
ML	machine learning
MSE	mean square error
NLARX	multivariable non-linear autoregressive with exogenous input
PID	proportional–integral–derivative
PIINN	physics informed integral neural network
<i>Symbols</i>	
n	sample size
y_i	the i^{th} predicted value
\hat{y}_i	the i^{th} actual value

1. INTRODUCTION

Dynamic modelling of CO₂ capture is important to support the deployment of capture technologies, particularly when integrated with power plants or combined heat and power (CHP) plants. The operation of these plants is dynamic due to variations in electricity and heat demand, leading to significant fluctuations in flue gas (FG) flowrate and composition. This can obviously affect the performance of downstream CO₂ capture processes [1, 2]. Steady-state models cannot capture these effects and are thus inadequate for tasks such as control design, real-time optimization and accurate performance assessment. Therefore, it is vital to develop dynamic models.

Dynamic models of MEA-based chemical absorption (MEA-CA) systems can be broadly categorized into

physics based models and machine learning (ML) based models [3]. Physics based models, built on mass transfer, heat transfer and chemical kinetics, are high-fidelity but computationally intensive and require substantial domain expertise [4], which will hinder their real-time applications, such as advanced control design and optimization. ML models offer a promising alternative due to their lower computational cost, demonstrating strong potential for real-time applications [4].

There are some studies that have explored the use of ML models in dynamic CO₂ capture systems by MEA-CA [4-8]. Some are used for system identification of control design. For example, Manaf et al. developed a multivariable non-linear autoregressive model with exogenous input (NLARX) [5]. The inputs considered included FG flowrate, CO₂ concentration (CO₂vol%) in FG, lean solvent flowrate and reboiler duty. The outputs included CO₂vol% at absorber outlet gas, CO₂vol% at top desorber, and top desorber flowrate. The model was validated using the absolute percentage error (APE), producing an APE of 0.034 for the CO₂ capture rate and 0.012–0.064 for the energy penalty. Sha et al. developed and compared nonlinear autoregressive neural network with exogenous input (NARX-NN), integral neural network (INN) and physics informed integral neural network (PIINN) [6]. The considered inputs included FG flowrate, FG CO₂vol%, lean solvent flowrate and reboiler duty. The outputs included CO₂ capture rate and the reboiler temperature. The results showed that, for these two outputs, the mean absolute percentage errors (MAPEs) were 13.2-20.9% and 0.1-98.3% for NARX-NN, 1.4-32.1% and 0.1-0.7% for INN, and 1.1-3.7% and 0.02-0.3% for PIINN, demonstrating that PIINN provides the most accurate predictions.

Some ML models are used for accurate assessment of CO₂ capture performance. For example, Li et al. first developed a bootstrap aggregated-neural network (BA-NN) model [4]. The considered inputs included FG flowrate, FG CO₂vol%, FG pressure, FG temperature, lean solvent flowrate, MEA concentration and the temperature of lean solvent. The outputs included the amount of captured CO₂ and CO₂ capture rate. Li et al. further developed a bootstrap aggregated extreme learning machine (BA-ELM) model [7] and a deep belief network (DBN) model by using the same input and output parameters [8]. The results showed that the mean square errors (MSEs) are 0.01-0.0771 kg/s and 0.001-0.2 % for the amount of captured CO₂ and CO₂ capture rate, respectively.

For the development of ML models, the selection of input features and the determination of outputs are

crucial [3]. The improper selected input features can lead to poor model accuracy and the improper outputs will make the model unrealistic and unable to be used since ML models can only provide results for explicitly specified outputs. There are various applications of dynamic models, which necessitate different inputs and outputs. While ML models have been applied to some applications [4-8], others remain unexplored. In addition, there has been no holistic study on what should be considered as inputs and outputs for different applications.

To bridge the existing knowledge gaps, this work aims to investigate the selection of input features and outputs for developing ML models and evaluate the capability of using ML approaches to develop dynamic models for different purposes. This work will provide guidance and insights into how to choose inputs and outputs for developing ML models of CO₂ capture.

2. APPLICATIONS OF DYNAMIC MODELS AND CURRENT USE OF ML MODELS IN CO₂ CAPTURE

2.1 Identifying the applications of dynamic models

Based on the literature review, there exist various applications of dynamic CO₂ capture models, such as control design and operation optimization, which can be categorized into four key cases.

Case 1: system identification for control development. In order to develop an effective control system, it is first crucial to understand the dynamic behavior of CO₂ capture system. Therefore, dynamic models need to be developed, known as system identification, to well represent the underlying dynamics. For the system identification of MEA-CA, some dynamic models have been developed using FG flowrate, lean solvent flowrate and reboiler duty as inputs, with CO₂ capture rate and reboiler temperature as outputs [9]. Such dynamic models could be deployed to design control systems with the objective of controlling the CO₂ capture rate.

Case 2: system monitoring and diagnosis. During the operation of the capture process, it is vital for operators to detect faults, such as sensor drift, actuator malfunctions and process anomalies, assess controller effectiveness, and maintain reliable operation. To achieve this, dynamic models can be developed as soft sensors to generate the reference manipulated variables and compare them with actual control actions. To ensure a reliable operation, the control system is normally designed to maintain a consistent CO₂ capture rate [10]. Some dynamic models have been developed for MEA-CA

to study the regulation of lean solvent flowrate and reboiler duty to ensure a constant CO₂ capture rate under the disturbance of FG flowrate [11]. This dynamic model could be deployed in real-time monitoring dashboards as a reference line to reveal hidden inefficiencies or early-stage faults.

Case 3: operation optimization. When CO₂ is integrated with energy-generating systems, such as CHP plants, there is growing interest in optimizing their dynamic operation. To support optimization, dynamic models of CO₂ capture are needed as surrogates within the process of optimization and further decision-making. Flexible operation might require rapid adjustment of the capture rate, responding to fluctuating heat demand, electricity prices and regulatory requirements for CO₂ emissions [12]. Some dynamic models have been developed for MEA-CA to track the desired CO₂ capture rate γ in a reasonable range (such as 50%-95%), under the disturbance of FG flowrate, by adjusting lean solvent flowrate and reboiler duty [13].

Case 4: system performance estimation. Dynamic models could provide more accurate performance metrics than steady state models, which can offer useful insights and thus are valuable for decision-makers and policymakers. There exist some dynamic models for MEA-CA, which were developed to examine the CO₂ capture feasibility and capability in waste or biomass CHP plants, in which CO₂ was only captured seasonally when there was excess heat from the plant [10].

2.2 Selecting inputs and outputs for ML modelling

After defining the application cases of dynamic CO₂ capture models, expected outputs and key input features for ML modelling must be selected, as summarized in Tab. 1. Before that, ML model development is examined to identify knowledge gaps. Based on literature, ML models have been applied to system identification (Case 1) [5, 6] and system performance estimation (Case 4) [4, 7, 8], but there is a gap in ML applications for system monitoring and diagnosis (Case 2) and operation optimization (Case 3). Therefore, Case 1 and Case 4 will be introduced first, followed by Case 2 and Case 3.

Tab. 1 Inputs and outputs of different cases

Cases	Key inputs	Expected outputs
Case 1	<ul style="list-style-type: none"> • FG flowrate • FG CO₂vol% • Lean flowrate • Reboiler duty 	<ul style="list-style-type: none"> • CO₂ capture rate • Reboiler temperature
Case 2	<ul style="list-style-type: none"> • FG flowrate • FG CO₂vol% 	<ul style="list-style-type: none"> • Reboiler duty • Lean flowrate • Electricity consumption

	<ul style="list-style-type: none"> • Constant CO₂ capture rate targets 	<ul style="list-style-type: none"> • Cooling water flowrate • Real-time CO₂ capture rate
Case 3	<ul style="list-style-type: none"> • FG flowrate • FG CO₂vol% • Varied CO₂ capture rate targets 	<ul style="list-style-type: none"> • Reboiler duty • Lean flowrate • Energy penalty
Case 4	<ul style="list-style-type: none"> • FG flowrate • FG CO₂vol% • Available reboiler duty 	<ul style="list-style-type: none"> • CO₂ capture amount • CO₂ capture rate • Energy penalty

For Case 1, to apply ML models in control development, the selection of model inputs and outputs must align with real disturbances and control actions. Since controlling the CO₂ capture rate is a common objective in dynamic operation, the ML model should be capable of predicting CO₂ capture rate in response to disturbances such as FG flowrate and CO₂vol%, given known control inputs like lean solvent flowrate and reboiler duty. Consistent with previous studies [5, 6, 9], typical inputs include FG flowrate, FG CO₂vol%, lean solvent flowrate, and reboiler duty. CO₂ capture rate and reboiler temperature are normally employed as outputs. For Case 4, the current ML model from Li et al. [4, 7, 8] included many input features, some of which are not essential and may unnecessarily increase model complexity. For example, FG pressure and temperature are often controlled and remain stable in the process of CO₂ capture from CHP plants [14]. If solvent loss can be neglected, the lean solvent MEA concentration is also stable. The main process inputs that undergo frequent time-variations are FG flowrate, FG CO₂vol%, and available reboiler duty. For output, in addition to CO₂ capture amount and CO₂ capture rate [4, 7, 8], the key performance, energy penalty is also included in this work.

For Case 2, in addition to FG flowrate and CO₂vol%, the constant CO₂ capture rate target is also included as input in this work. The expected outputs include key manipulated variables (lean solvent flowrate, reboiler duty) and key utilities (electricity consumption and cooling water flowrate). In addition, the real-time CO₂ capture rate is also selected as an output and compared with the measured value for fault detection, as with manipulated variables. For Case 3, similar to Case 2, the varied CO₂ capture rate target is also included as input. In addition to key manipulated variables, the energy penalty is also selected as the output.

3. METHODOLOGY

To develop ML models for MEA-CA systems, both accurate data input and ML models are essential. This

section first introduced the data generation process for different cases from physical modelling. Then three ML approaches were presented, followed by the performance metrics used to validate and compare the models.

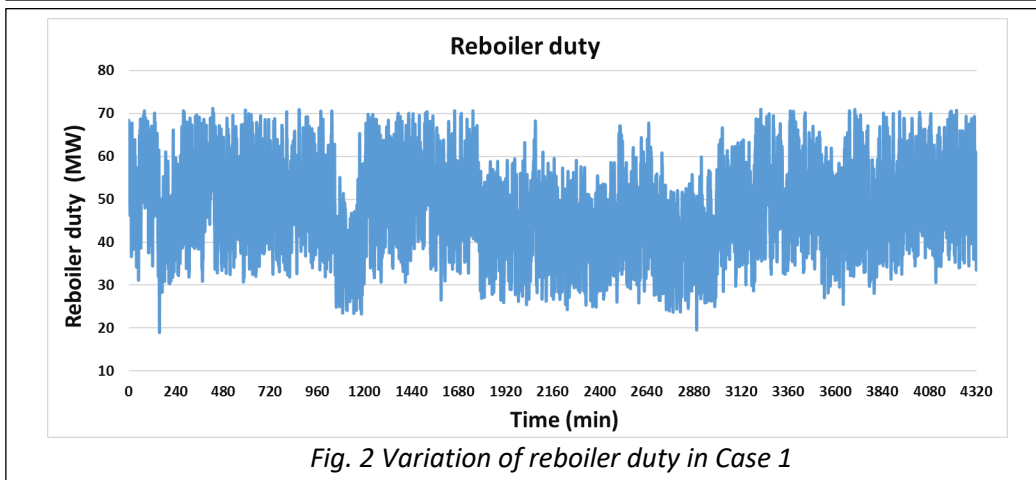
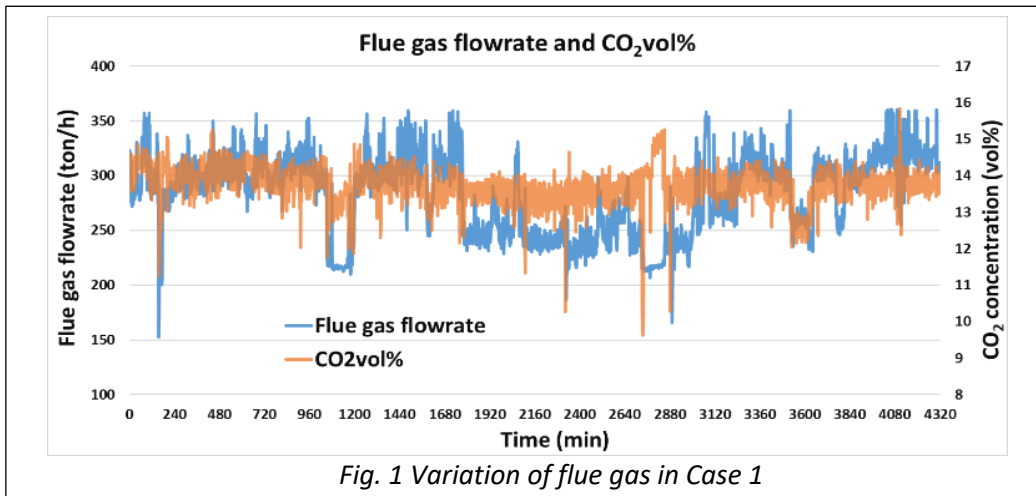
3.1 Data generation

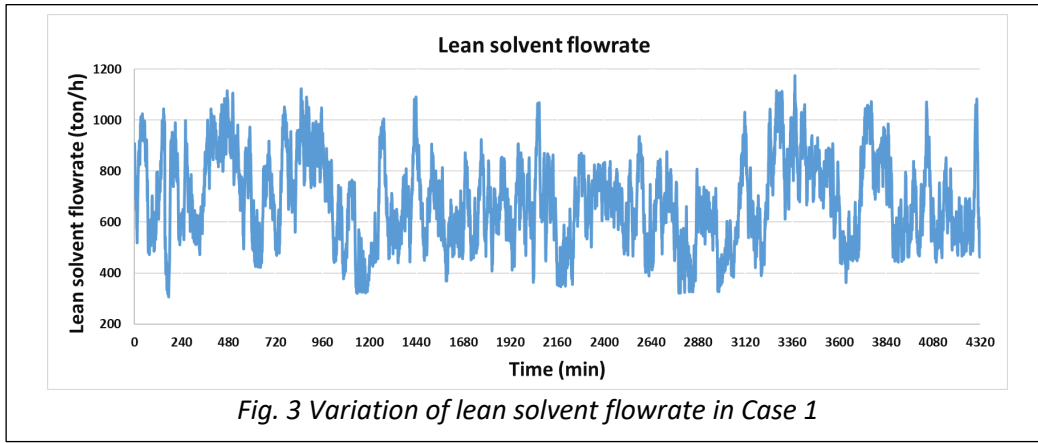
To generate data for ML models training and validation, dynamic simulations of MEA-CA were conducted using a physical model developed in Aspen HYSYS Dynamics V12.1. Detailed model development and validation can be found in a previous study [15]. Different simulations were conducted for the four different cases identified in Section 2. For Case 1, the simulation was conducted for the open-loop process without any controllers. For Case 2, Case 3 and Case 4, the simulation was conducted for the closed-loop process with controllers, which input-output behaviors show both the system dynamics and how the controller reacts.

The primary inputs included both dynamic and constant parameters. There were some constant input

parameters that were the same for all four cases. They included FG temperature (47°C), initial pressure (143 kPa), and the initial conditions of the lean solvent (41°C, 107 kPa, 30 wt.% MEA and 0.287 lean loading).

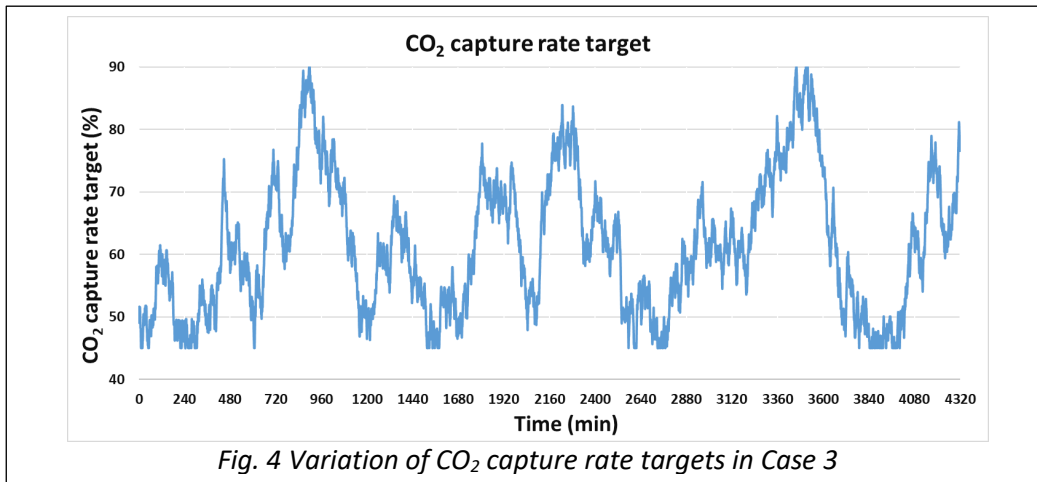
For dynamic inputs, in Case 1, FG flowrate and CO₂vol% were obtained from a real waste CHP plant, which covered three days in 2019, as shown in Fig. 1. The FG flowrate and CO₂vol% varied in ranges of 150-360 ton/h and 9.6-15.8 vol%, respectively. The time resolution was 1 minute. Based on the actual FG flowrate and CO₂vol%, a range of reboiler duty can be obtained by using a range of possible capture rates (45-90%) and an average energy penalty (4.5 MJ/kg), based on which the dynamic input signal for reboiler duty (Fig. 2) was generated. The dynamic input signal for lean solvent flowrate (Fig. 3) was generated based on the actual FG flowrate and a physically realistic liquid-to-gas ratio (L/G) range of 1.5-3.5 (mass basis) in MEA-CA systems [16]. This range maintains safe and stable hydraulic operation, ensuring adequate CO₂ capture efficiency but at the same time avoiding flooding risks [16].





In Case 2 and Case 3, FG flowrate and CO₂vol% were same as Case 1. The constant CO₂ capture rates targets were 70%, 80% and 90% in Case 2; and the varied CO₂ capture rate signal was generated randomly in the range of 45%-90% (Fig. 4) in Case 3, since it was assumed that

the CO₂ capture system was not operating when CO₂ capture rate was less than 45%. To achieve those CO₂ capture rates targets, the lean solvent flowrate and reboiler duty were manipulated by adding proportional-integral-derivative (PID) controllers.



In Case 4, FG (flowrate and CO₂vol%) and reboiler duty were determined by optimizing the operation of the CHP plant integrated with CO₂ capture. Based on the two operating strategies in [17], the corresponding FG and reboiler duty were shown in Fig. 5 based on optimization in 3600 minutes. To alleviate the fluctuation of CO₂ absorption efficiency, the lean solvent flowrate was manipulated by PID controllers to maintain the desired reboiler temperature and thus the desired CO₂ lean loading.

3.2 Machine learning approaches

Three ML approaches were selected in this work.

Informer is a deep neural network architecture designed for sequence modeling, which captures dependencies between input elements by assigning importance weights. It introduces a probabilistic sparse self-attention mechanism to reduce computational costs by focusing on the most informative queries [18]. This enables efficient processing of large-scale data and long

sequences. Therefore, Informer might be a useful tool for modeling the dynamic CO₂ capture process in CHP plants, given the inherent variability in CHP plant operations and the complex behavior of the MEA-CA system.

Long short-term memory network (LSTM) was proposed to address the issue of recurrent neural networks, namely vanishing gradient and thus poor ability to learn long-term dependencies [19]. It introduces memory cell units, which facilitate the retention of relevant information across long sequences and consist of three gates, including input gate, forgetting gate and output gate. This architecture enables LSTM to capture both short-term and long-term dependencies, possibly making it an effective tool for dynamic systems with delayed responses. Therefore, LSTM might be suited for modeling the dynamic CO₂ capture process in CHP plants, in which the MEA-CA system exhibits delayed responses to variations in operating conditions.

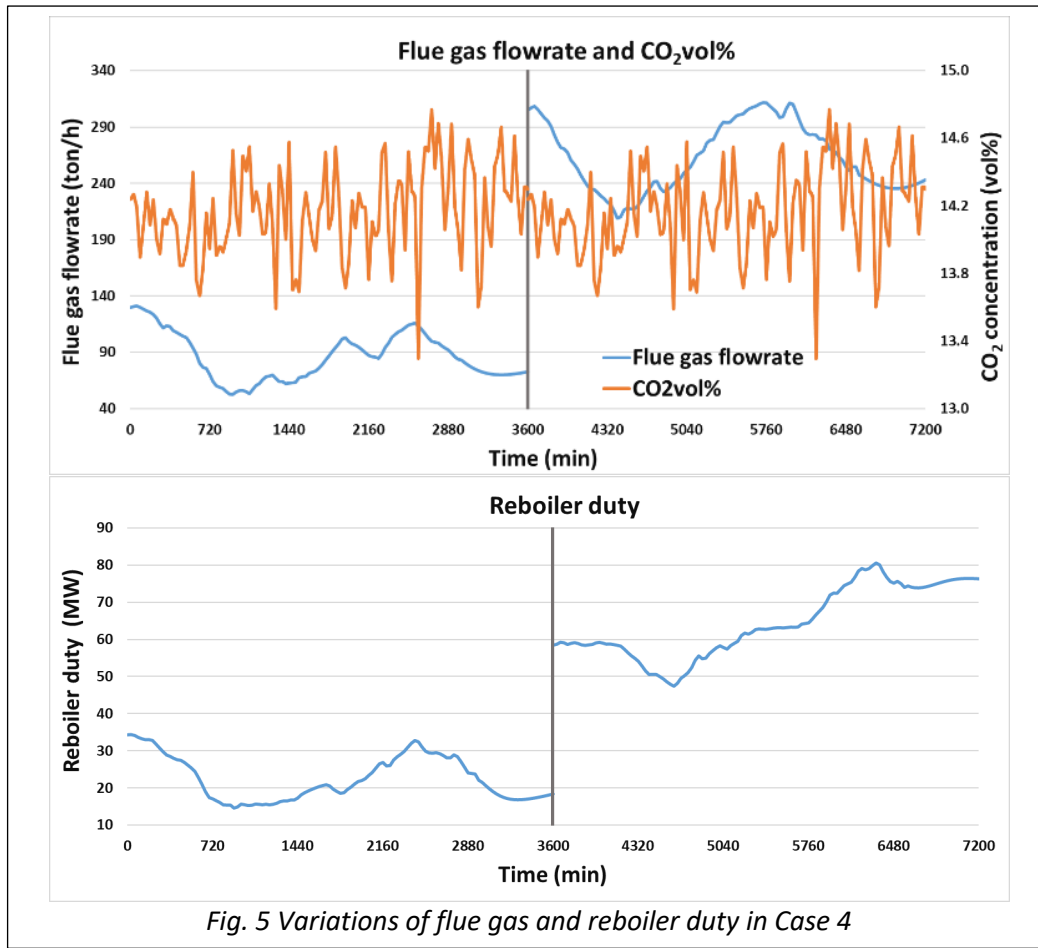


Fig. 5 Variations of flue gas and reboiler duty in Case 4

Back propagation neural network (BPNN) is a multilayer feedforward network, with simpler architecture than Informer and LSTM. In a neural network, each layer is composed of neurons that are interconnected. The layers work together to process data through a series of transformations. The learning process involves signal forward propagation and error back propagation. The core is to constantly adjust the weights and biases of the neurons in each layer to minimize the error. Although BPNN is not inherently designed for sequence modeling, time-series data can be transformed into a static tabular format compatible by employing a sliding window technique [20]. BPNN has high nonlinear mapping and good generalization ability using the global approximation method. Therefore, it was selected due to the high nonlinearity of the MEA-CA system and the wide operation ranges of CHP plants. As a fundamental neural network model, BPNN also serves as a popular benchmark for evaluating more advanced approaches [21].

To compare the performance of ML models, the mean absolute percentage error (MAPE) and mean

absolute error (MAE) were employed as performance metrics, defined in Equations 1 and 2, respectively.

$$MAPE = \frac{1}{n} \sum_{i=1}^n \left| \frac{y_i - \hat{y}_i}{\hat{y}_i} \right| \times 100\% \quad (1)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i| \quad (2)$$

where n is the sample size; y_i is the i^{th} predicted value; and \hat{y}_i is the i^{th} actual value.

The datasets generated by the physical models, including input and output variables, were divided into training data (70%), validation data (10%), and testing data (20%). The performance metrics were calculated based on testing data.

4. RESULTS

4.1 Case 1: system identification for control development

Tab. 2 presents the performance metrics of the three ML models for Case 1. Overall, all models achieve acceptable performance. In comparison, Informer shows the best performance. BPNN is superior to LSTM when it comes to CO₂ capture rate, while LSTM is superior to BPNN for the reboiler temperature.

Tab. 2 Prediction accuracy for Case 1

ML-models	CO ₂ capture rate		Reboiler temperature
	MAPE (%)	MAE	MAE (°C)
Informer	3.68	0.025	0.06
LSTM	7.42	0.053	0.09
BPNN	5.53	0.038	1.05

4.2 Case 2: system monitoring and diagnosis

Tab. 3 presents the performance metrics of the three ML models for Case 2. Overall, all models achieve satisfactory performance, with MAPE values below 5%. In comparison, Informer consistently shows the best performance across all five outputs. The comparison between LSTM and BPNN varies with the outputs. LSTM can show lightly better performance (such as power consumption), or worse performance (such as lean solvent) than BPNN. In addition, the prediction errors of LSTM/BPNN are more than twice as high as Informer's for most of the predicted outputs.

Tab. 3 Prediction accuracy for Case 2

ML-models	Reboiler duty		Lean solvent	
	MAPE (%)	MAE (MW)	MAPE (%)	MAE (ton/h)
Informer	0.89	0.43	1.33	12.6
LSTM	2.98	1.60	3.84	36.6
BPNN	2.82	1.54	2.89	28.2

ML-models	Power consumption		Cooling water		CO ₂ capture rate	
	MAPE (%)	MAE (kW)	MAPE (%)	MAE (ton/h)	MAPE (%)	MAE
Informer	1.08	0.26	1.09	34	2.97	0.024
LSTM	2.39	0.58	1.67	53	4.63	0.038
BPNN	2.50	0.67	2.97	101	3.03	0.024

4.3 Case 3: operation optimization

Tab. 4 presents the performance metrics of the three ML models for Case 3. Overall, all models achieve acceptable performance, with most MAPE values below 5%, except when modeling the regulation of lean solvent flowrate using LSTM. In comparison, same as Case 2, Informer consistently shows the best performance across all three outputs, particularly excelling in predicting reboiler duty and energy penalty. BPNN shows overall better performance than LSTM.

Tab. 4 Prediction accuracy for Case 3

ML-models	Reboiler duty		Lean solvent		Energy penalty	
	MAPE (%)	MAE (MW)	MAPE (%)	MAE (ton/h)	MAPE (%)	MAE (MJ/kg)
Informer	0.90	0.40	3.53	24.9	0.64	0.03
LSTM	3.82	1.54	5.78	41.7	4.64	0.21
BPNN	3.84	1.57	3.57	25.6	2.22	0.10

4.4 Case 4: system performance estimation

Tab. 5 presents the performance metrics of the three ML models for Case 4. Overall, all models demonstrate satisfactory performance, with MAPE values below 5% for all outputs. Unlike the previous cases, no single model performs best across all outputs. Instead, the performance varies depending on the target outputs. Informer yields the most accurate predictions for CO₂ capture rate; LSTM slightly outperforms the others for the energy penalty, while BPNN shows the lowest error for CO₂ capture amount.

Tab. 5 Prediction accuracy for Case 4

ML-models	CO ₂ capture amount		Energy penalty		CO ₂ capture rate	
	MAPE (%)	MAE (ton/h)	MAPE (%)	MAE (MJ/kg)	MAPE (%)	MAE
Informer	3.26	1.15	1.52	0.08	0.52	0.005
LSTM	4.27	1.37	1.02	0.05	1.75	0.017
BPNN	2.57	0.72	3.79	0.19	2.42	0.023

5. DISCUSSION

This study investigated the application of ML-based models for the dynamic modeling of CO₂ capture in CHP plants. It has been found that even though Informer exhibits high accuracy, no single model consistently outperforms the others across all cases and target outputs, but each model demonstrated unique strengths that make it well-suited for specific applications. For example, when employing Informer, the model excels in capturing long-term temporal dependencies and dynamic system interactions, making it the most effective choice for supporting operation optimization and planning tasks. While the BPNN model shows superior performance for variables dominated by nonlinear input-output relationships, such as CO₂ capture amount in the system performance estimation task. For the same application, ML model performance also varies with the target outputs, even though those target outputs are theoretically related, such as CO₂ capture amount and CO₂ capture rate in Case 4. The ML model performance may stem from a combination of factors, including the complexity of nonlinear input-output relationships, model's sensitivity to dataset size and the characteristics of each target output. These findings provided valuable guidance for practical applications. The model selection must be tailored to the specific characteristics of the target variables and operating cases, as no single model is universally ideal.

Even though four key cases are identified, their input and output selections may also change depending on the detailed applications. For example, when the control target is not CO₂ capture rate but the energy penalty, the

lean loading and reboiler temperature should be employed as input and the energy penalty must be the output.

6. CONCLUSIONS

There exist various applications for the dynamic operation of CO₂ capture, and accurately modelling dynamic CO₂ capture is essential for process control, optimization and estimation. This study first reviewed the literature to identify the needs for different applications of dynamic modelling. Then, by employing ML approaches, including Informer, LSTM, and BPNN, three models were developed based on the dataset from rigor simulations of a waste CHP plant with CO₂ capture. The key findings were summarized as follows:

- It is essential to identify specific needs for different dynamic modelling applications.
- ML modelling is a feasible method, which can achieve satisfactory accuracy for all cases, most MAPEs below 5%.
- For each case, employing different ML approaches results in different performance. Even though Informer exhibits high accuracy, no single model consistently outperforms the others across all cases.

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